

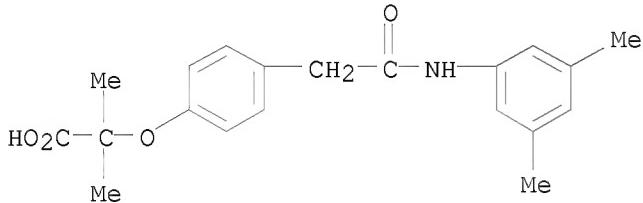
10/598,854

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> s efaproxiral/cn  
L1 1 EFAPROXIRAL/CN

=> d  
THE ESTIMATED COST FOR THIS REQUEST IS 2.10 U.S. DOLLARS  
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2010 ACS on STN  
RN 131179-95-8 REGISTRY  
ED Entered STN: 28 Dec 1990  
CN Propanoic acid, 2-[4-[2-[(3,5-dimethylphenyl)amino]-2-oxoethyl]phenoxy]-2-methyl- (CA INDEX NAME)  
OTHER NAMES:  
CN 2-[4-[[[(3,5-Dimethylphenyl)amino]carbonyl]methyl]phenoxy]-2-methylpropionic acid  
CN Efaproxiral  
CN RSR 13  
MF C20 H23 N O4  
CI COM  
SR CA  
LC STN Files: ADISINSIGHT, ADISNEWS, ANABSTR, BEILSTEIN\*, BIOSIS, BIOTECHNO, CA, CAPLUS, CASREACT, CHEMCATS, CIN, DDFU, DRUGU, EMBASE, IMSDRUGNEWS, IMSPATENTS, IMSRESEARCH, IPA, MEDLINE, MRCK\*, PROMT, PROUSDDR, RTECS\*, SYNTHLINE, TOXCENTER, USAN, USPAT2, USPATFULL  
(\*File contains numerically searchable property data)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

110 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
112 REFERENCES IN FILE CAPLUS (1907 TO DATE)

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	8.09	8.31

FILE 'CAPLUS' ENTERED AT 15:21:36 ON 19 MAY 2010  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
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FILE COVERS 1907 - 19 May 2010 VOL 152 ISS 21  
FILE LAST UPDATED: 18 May 2010 (20100518/ED)  
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2010  
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Apr 2010

CAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2010.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

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      4990624 PREP/RL
L2          14 131179-95-8/PREP
                  (131179-95-8 (L) PREP/RL)

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      334074 PUR/RL
L3          0 131179-95-8/PUR
                  (131179-95-8 (L) PUR/RL)

=> s l2 and ( water or ethanol or acetone)
      3071740 WATER
      364953 ETHANOL
      208948 ACETONE
L4          7 L2 AND ( WATER OR ETHANOL OR ACETONE)

=> s l4 and py<2005
      25158174 PY<2005
L5          5 L4 AND PY<2005

=> l-5 ibib abs hitstr
1-5 IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (>).

=> d l-5 ibib abs hitstr
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10/923,271

THE ESTIMATED COST FOR THIS REQUEST IS 29.05 U.S. DOLLARS  
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L5 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2010 ACS on STN  
ACCESSION NUMBER: 1995:758997 CAPLUS  
DOCUMENT NUMBER: 124:55568  
ORIGINAL REFERENCE NO.: 124:10501a,10504a  
TITLE: Substituted 2-methyl-2-phenoxypropionic acid derivatives as allosteric hemoglobin modifiers to decrease oxygen affinity in blood  
INVENTOR(S): Abraham, Donald J.; Mahrani, Mona; Mehanna, Ahmed; Randad, Ramnarayan; Joshi, Gajanan S.; Panikker, Jayashree  
PATENT ASSIGNEE(S): Center for Innovative Technology, USA  
SOURCE: U.S., 24 pp. Cont.-in-part of U.S. 5,290,803.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 8  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5432191	A	19950711	US 1993-101501	19930730 <--
US 5049695	A	19910917	US 1990-478848	19900212 <--
US 5122539	A	19920616	US 1991-702947	19910520 <--
US 5382680	A	19950117	US 1991-722382	19910626 <--
US 5290803	A	19940301	US 1993-6246	19930119 <--
US 5731454	A	19980324	US 1995-374206	19950118 <--
US 5591892	A	19970107	US 1995-451658	19950530 <--
US 5648375	A	19970715	US 1995-478372	19950607 <--
US 5661182	A	19970826	US 1995-478108	19950607 <--
US 5677330	A	19971014	US 1995-478371	19950607 <--
US 5705521	A	19980106	US 1995-482808	19950607 <--
US 5927283	A	19990727	US 1997-848485	19970508 <--
US 5872282	A	19990216	US 1998-41595	19980313 <--
PRIORITY APPLN. INFO.:			US 1990-478848	A2 19900212
			US 1990-623346	B1 19901207
			US 1991-702947	A2 19910520
			US 1991-722382	A2 19910626
			US 1993-6246	A2 19930119
			US 1992-885721	A1 19920518
			US 1993-101501	A2 19930730
			US 1993-127587	B1 19930928
			US 1995-374206	A3 19950118
			US 1995-478371	A3 19950607

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 124:55568

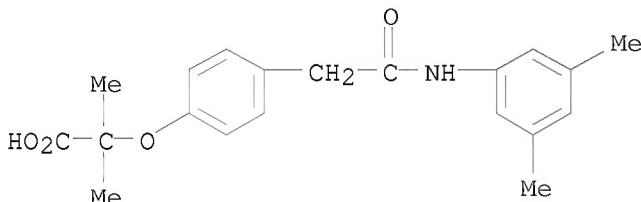
AB A family of compds. R2XYZC6H4R1 where R2 is a substituted or unsubstituted aromatic compound, or a substituted or unsubstituted alkyl ring compound, or a substituted or unsubstituted phthalimide compound that incorporates X and Y where X is a carbonyl, Y is a nitrogen and R2 completes the phthalimide compound by being bonded to both X and Y, and where X, Y, and Z are CH<sub>2</sub>, NH, S, SO<sub>2</sub>, CO, O or N with the caveat that the X, Y, and Z moieties are each different from one another, and where R1 has the formula: OCR<sub>3</sub>R<sub>4</sub>CO<sub>2</sub>R<sub>5</sub> where R1 can be connected to any position on the Ph ring, and R3 and R4

are hydrogen, halogen, Me, Et, Pr, iso-Pr, neopentyl, Bu, or substituted or unsubstituted aryl groups and these moieties may be the same or different, or alkyl moieties as part of an aliphatic ring connecting R3 and R4, and R5 is a hydrogen, halogen, C1-3 loweralkyl, or a salt cation, has been found to be useful for right-shifting Hb towards a low oxygen affinity state. The compds. are capable of acting on Hb in whole blood. In addition, the compds. can maintain the oxygen affinity in blood during storage and can restore the oxygen affinity of outdated blood. Thus, e.g., treatment of 4-HOC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>CO<sub>2</sub>H with SOC<sub>12</sub> and 3,5-dichloroaniline afforded the intermediate 4-HOC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>CONHC<sub>6</sub>H<sub>3</sub>Cl<sub>2</sub>-3,5; O-alkylation of the latter with acetone/CHCl<sub>3</sub> afforded 4-(HO<sub>2</sub>CCMe<sub>2</sub>O)C<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>CONHC<sub>6</sub>H<sub>3</sub>Cl<sub>2</sub>-3,5 which exhibited a P50 (mm Hg) of 87 for oxygen dissociation of normal Hb in intact human red blood cells vs. 27 for the red blood cells alone (P50 = the pressure when the scanned Hb sample is 50% saturated with oxygen).

IT 131179-95-8P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (substituted 2-methyl-2-phenoxypropionic acid derivs. as allosteric Hb modifiers to decrease oxygen affinity in blood)

RN 131179-95-8 CAPLUS

CN Propanoic acid, 2-[4-[2-[(3,5-dimethylphenyl)amino]-2-oxoethyl]phenoxy]-2-methyl- (CA INDEX NAME)



OS.CITING REF COUNT: 12 THERE ARE 12 CAPLUS RECORDS THAT CITE THIS RECORD (16 CITINGS)  
 REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

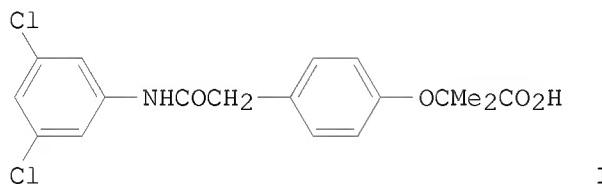
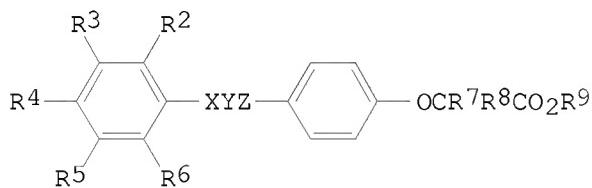
L5 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1993:495107 CAPLUS  
 DOCUMENT NUMBER: 119:95107  
 ORIGINAL REFERENCE NO.: 119:17137a,17140a  
 TITLE: Preparation of phenoxymethylpropionate derivatives as allosteric hemoglobin modifiers to decrease oxygen affinity in blood  
 INVENTOR(S): Abraham, Donald J.; Mahran, Mona; Mehanna, Ahmed; Randad, Ramnarayan  
 PATENT ASSIGNEE(S): Center for Innovative Technology, USA  
 SOURCE: PCT Int. Appl., 67 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 8  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9220335	A1	19921126	WO 1992-US4229	19920519 <--
W: CA, JP RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE				
US 5122539	A	19920616	US 1991-702947	19910520 <--
US 5248785	A	19930928	US 1992-885721	19920518 <--
EP 585366	A1	19940309	EP 1992-912561	19920519 <--
EP 585366	B1	20040428		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, SE				
JP 07508973	T	19951005	JP 1993-500270	19920519 <--
JP 3023423	B2	20000321		
CA 2109575	C	20000201	CA 1992-2109575	19920519 <--
AT 265208	T	20040515	AT 1992-912561	19920519 <--
PRIORITY APPLN. INFO.:			US 1991-702947	A 19910520
			US 1992-885721	A 19920518
			US 1990-478848	A2 19900212
			WO 1992-US4229	W 19920519

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 119:95107

GI



AB Title compds. I (R2-R6 = H, halo, (substituted) C1-3 alkyl, C1-3 alkyl ether or ester, alkyl moieties of aromatic or aliphatic ring incorporating 2 of R2-R6 site; R7, R8 = H, Me, Et, etc.; R9 = H, halo, (substituted) C1-3 alkyl, cation salt; X, Y, Z = CH<sub>2</sub>, CO, NH, O) are prepared as allosteric Hb modifiers to decrease O affinity in blood. 4-HOC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>CO<sub>2</sub>H was refluxed with excess SOCl<sub>2</sub>, then reacted for 2 h with 3,5-C<sub>12</sub>C<sub>6</sub>H<sub>3</sub>NH<sub>2</sub> to give after workup II, which showed a decrease in Hb-O affinity (i.e., increase in P<sub>50</sub> value of 87 from control 19).

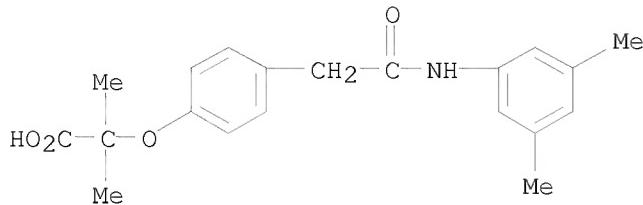
IT 131179-95-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, for lowering oxygen affinity to Hb in blood)

RN 131179-95-8 CAPLUS

CN Propanoic acid, 2-[4-[2-[(3,5-dimethylphenyl)amino]-2-oxoethyl]phenoxy]-2-

methyl- (CA INDEX NAME)



OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD  
 (5 CITINGS)  
 REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 1993:45721 CAPLUS  
 DOCUMENT NUMBER: 118:45721  
 ORIGINAL REFERENCE NO.: 118:8119a,8122a  
 TITLE: Allosteric hemoglobin modifiers useful for decreasing oxygen affinity and preserving oxygen carrying capability of stored blood  
 INVENTOR(S): Abraham, Donald J.; Mahrani, Mona; Mehanna, Ahmed; Randad, Ramnarayan  
 PATENT ASSIGNEE(S): Center for Innovative Technology, USA  
 SOURCE: U.S., 20 pp. Cont.-in-part of U.S. 5,049,695.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 8  
 PATENT INFORMATION:

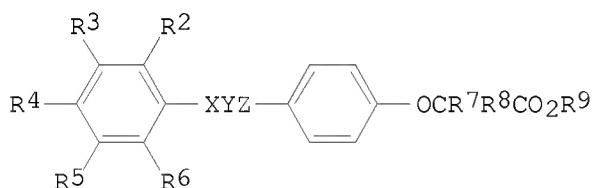
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US 5122539	A	19920616	US 1991-702947	19910520 <--
US 5049695	A	19910917	US 1990-478848	19900212 <--
CA 2051693	A1	19910813	CA 1991-2051693	19910206 <--
CA 2051693	C	20050607		
US 5248785	A	19930928	US 1992-885721	19920518 <--
WO 9220335	A1	19921126	WO 1992-US4229	19920519 <--
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RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE				
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EP 585366	B1	20040428		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, SE				
JP 07508973	T	19951005	JP 1993-500270	19920519 <--
JP 3023423	B2	20000321		
CA 2109575	C	20000201	CA 1992-2109575	19920519 <--
EP 1236711	A2	20020904	EP 2002-12781	19920519 <--
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AT 260886	T	20040315	AT 2002-12781	19920519 <--
AT 265208	T	20040515	AT 1992-912561	19920519 <--

EP 1468680	A2	20041020	EP 2004-9908	19920519 <--
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ES 2223042	T3	20050216	ES 1992-912561	19920519
US 5250701	A	19931005	US 1993-6378	19930119 <--
US 5290803	A	19940301	US 1993-6246	19930119 <--
US 5432191	A	19950711	US 1993-101501	19930730 <--
US 5731454	A	19980324	US 1995-374206	19950118 <--
US 5591892	A	19970107	US 1995-451658	19950530 <--
US 5648375	A	19970715	US 1995-478372	19950607 <--
US 5661182	A	19970826	US 1995-478108	19950607 <--
US 5677330	A	19971014	US 1995-478371	19950607 <--
US 5705521	A	19980106	US 1995-482808	19950607 <--
US 5927283	A	19990727	US 1997-848485	19970508 <--
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		US 1990-478848	A2 19900212	
		US 1990-623346	A1 19901207	
		US 1991-702947	A2 19910520	
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		US 1992-885721	A 19920518	
		EP 1992-912561	A3 19920519	
		WO 1992-US4229	W 19920519	
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		US 1993-101501	A2 19930730	
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		US 1995-374206	A3 19950118	
		US 1995-478371	A3 19950607	

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 118:45721

GI



AB I (X,Y,Z = CH<sub>2</sub>, NH or O and R<sub>2</sub>-R<sub>6</sub> = e.g., H, halo, substituted or unsubstituted C<sub>1</sub>-3 allyl, R<sub>7</sub>, R<sub>8</sub> = H, Me or Et, R<sub>9</sub> = H, alkyl, or metal salt) are prepared and have the ability to maintain oxygen affinity in blood during storage and can restore the O affinity of outdated blood.  
 p-Acetaminophenol was treated with acetone and CHCl<sub>3</sub> in NaOH solution and the acetaminophenoxyethylpropionic acid obtained after acidification was hydrolyzed and later acylated with an acid chloride such as phenylacetyl chloride. The compds. showed O carrying properties of stored blood.

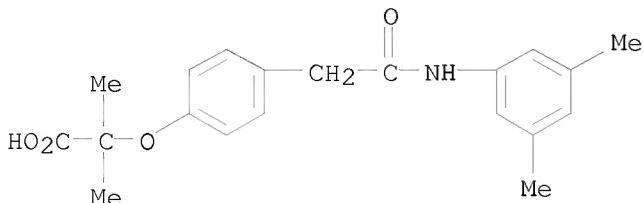
IT 131179-95-8P

RL: PREP (Preparation)

(preparation of, as allosteric Hb modifier for decreasing oxygen affinity

10/923,271

and preserving oxygen carrying properties)  
RN 131179-95-8 CAPLUS  
CN Propanoic acid, 2-[4-[2-[(3,5-dimethylphenyl)amino]-2-oxoethyl]phenoxy]-2-methyl- (CA INDEX NAME)

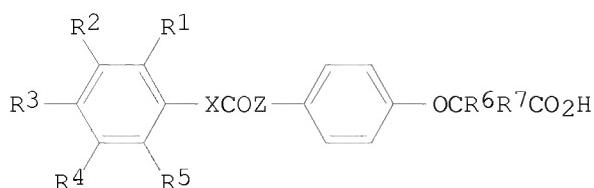


OS.CITING REF COUNT: 24 THERE ARE 24 CAPLUS RECORDS THAT CITE THIS RECORD (40 CITINGS)  
REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2010 ACS on STN  
ACCESSION NUMBER: 1991:655817 CAPLUS  
DOCUMENT NUMBER: 115:255817  
ORIGINAL REFERENCE NO.: 115:43485a, 43488a  
TITLE: Preparation of allosteric hemoglobin modifiers  
INVENTOR(S): Abraham, Donald J.; Mehanna, Ahmed; Randad, Ramnarayan; Mahrani, Mona  
PATENT ASSIGNEE(S): Center for Innovative Technology, USA  
SOURCE: PCT Int. Appl., 24 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 8  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9112235	A1	19910822	WO 1991-US833	19910206 <--
W: CA, JP				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				
US 5049695	A	19910917	US 1990-478848	19900212 <--
CA 2051693	A1	19910813	CA 1991-2051693	19910206 <--
CA 2051693	C	20050607		
EP 471811	A1	19920226	EP 1991-904612	19910206 <--
EP 471811	B1	19951227		
R: DE, FR, GB, IT				
JP 04506812	T	19921126	JP 1991-504932	19910206 <--
JP 3023422	B2	20000321		
PRIORITY APPLN. INFO.:			US 1990-478848 A	19900212
			WO 1991-US833 W	19910206

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT  
OTHER SOURCE(S): CASREACT 115:255817; MARPAT 115:255817  
GI



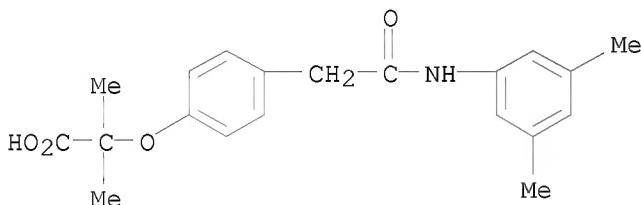
AB Title modifiers I [R1 - R5 = H, halo, (substituted) C1-3 alkyl; R6, R7 = H, Me; X, Z = CH<sub>2</sub>, NH, O, with the proviso that when X is CH<sub>2</sub>, Z is NH, when X is NH, Z is either CH<sub>2</sub> or O, and when X is O, Z is NH] are prepared NaOH was added to p-(AcNH)C<sub>6</sub>H<sub>4</sub>OH in acetone, followed by addition of CHCl<sub>3</sub>, to give after acidification with HCl the appropriate (acetaminophenoxy)methylpropionic acid, which was treated with KOH to give 4-(H<sub>2</sub>N)C<sub>6</sub>H<sub>4</sub>OCMe<sub>2</sub>CO<sub>2</sub>H, which was dissolved with stirring in aqueous NaOH, and to this solution was added PhCH<sub>2</sub>COCl to give I (R1-R5 = H, R6 = R7 = Me, X = CH<sub>2</sub>, Z = NH) (II). The biol. activities of II and addnl. I are given.

IT 131179-95-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, as allosteric Hb modifier)

RN 131179-95-8 CAPLUS

CN Propanoic acid, 2-[4-[2-[(3,5-dimethylphenyl)amino]-2-oxoethyl]phenoxy]-2-methyl- (CA INDEX NAME)

OS.CITING REF COUNT: 9 THERE ARE 9 CAPLUS RECORDS THAT CITE THIS RECORD  
(12 CITINGS)

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1991:81170 CAPLUS

DOCUMENT NUMBER: 114:81170

ORIGINAL REFERENCE NO.: 114:13837a,13840a

TITLE: Allosteric modifiers of hemoglobin. 1. Design, synthesis, testing, and structure-allosteric activity relationship of novel hemoglobin oxygen affinity decreasing agents

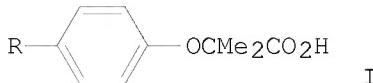
AUTHOR(S): Randad, Ramnarayan S.; Mahran, Mona A.; Mehanna, Ahmed S.; Abraham, Donald J.

CORPORATE SOURCE: Dep. Med. Chem., Virginia Common. Univ., Richmond, VA, 23298-0581, USA

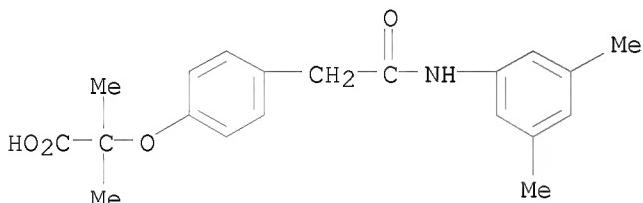
SOURCE: Journal of Medicinal Chemistry (1991), 34(2), 752-7

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 114:81170  
 GI



- AB Three isomeric series of 2-aryloxy-2-methylpropionic acids I ( $R = R_1CH_2CONH$ ,  $R_1CONHCH_2$ ,  $R_1NHCOCH_2$ ;  $R_1 = Ph$ , substituted phenyl) were prepared and studied for their ability to decrease the oxygen affinity of human Hb A. Structure-activity relationships are presented. Several of the new compds. were strong allosteric effectors of Hb. The two most active compds. are I ( $R = 3,5-R_2C_6H_3NHCOCH_2$ ;  $R_2 = Cl$ , Me) (II). Compared to other known potent allosteric effectors, II show greater activity. II also exhibit a right shift in the oxygen equilibrium curve when incubated with whole blood.
- IT 131179-95-8P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of, as allosteric effector of Hb)
- RN 131179-95-8 CAPLUS
- CN Propanoic acid, 2-[4-[2-[(3,5-dimethylphenyl)amino]-2-oxoethyl]phenoxy]-2-methyl- (CA INDEX NAME)



OS.CITING REF COUNT: 44 THERE ARE 44 CAPLUS RECORDS THAT CITE THIS RECORD (45 CITINGS)

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